MC simulations of i-TED 4π & background rejection studies

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The n_TOF Collaboration

European Research Council

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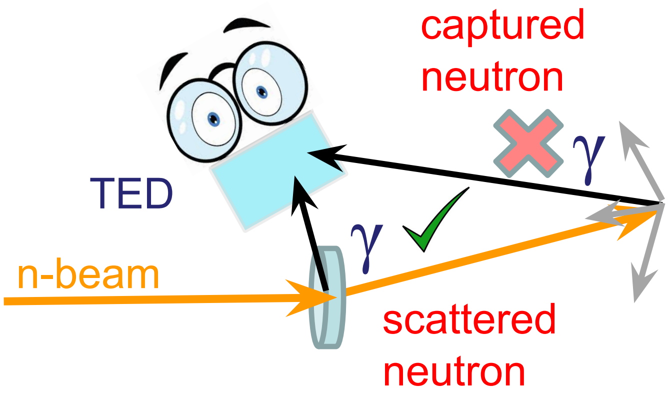
VNIVERSITAT DE VALÈNCIA

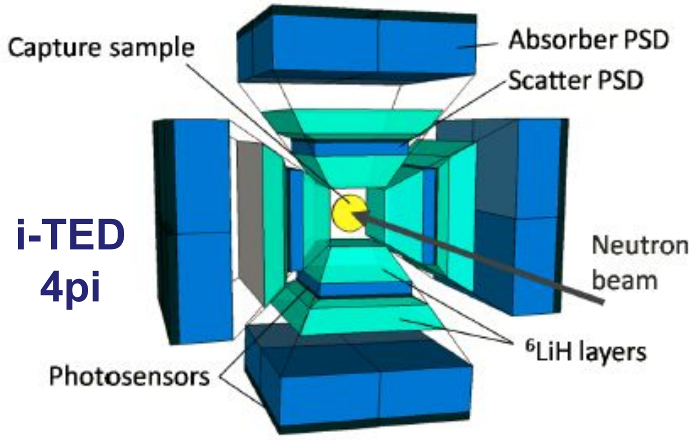
CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Outline

- **Introduction to i-TED and motivation**
- **MC simulation of i-TED: capture and background events**
  - i-TED Response to (n,g) and background
  - Imaging of (n,g) and background
- **Background rejection based on MC simulations**
  - Analytical imaging cuts: the λ parameter
  - (n,g)/background gain: i-TED vs C6D6
  - ML-based vs analytical background rejection
- **ML-based background rejection with i-TED 5.3 data**
- **Summary**

Motivation





- **i-TED Concept:** Combine TED & Compton imaging to reduce extrinsic neutron background
- **Plans for final i-TED-4pi**
  - Under development but not yet commissioned @ n_TOF → no experimental data of final detector
  - Commissioning and Se-79(n,g) measurement in 2021/22

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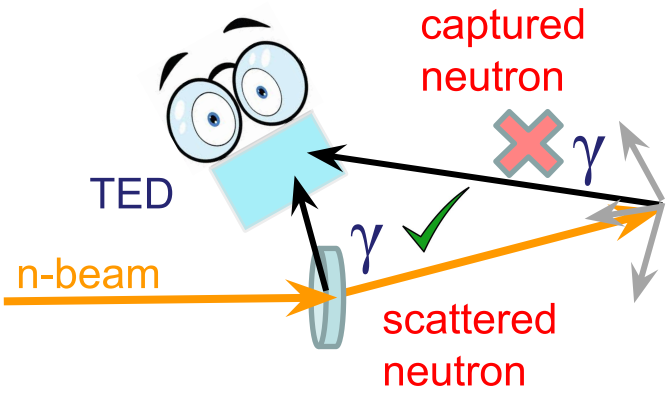

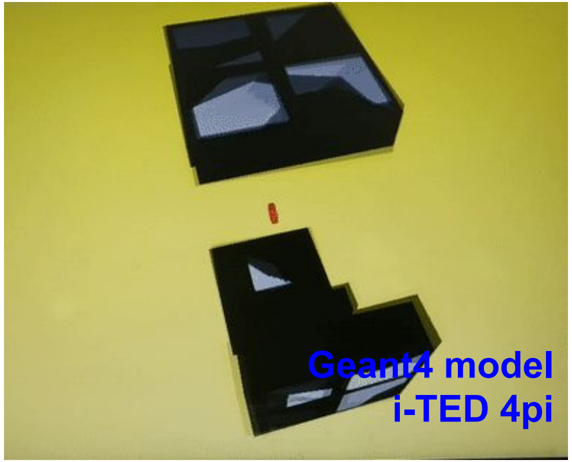

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- **Goal MC simulations:**
  - Optimization of crystal thickness, S-A distance,..
  - Counting rate estimates for Se-79(n,g)
  - Optimization of imaging and background rejection
  - Study of impact of experimental effects (resolution, backscattering, summing,...)
  - Understand results i-TED 5.3 commissioning @ n_TOF and i-TED5 @ IFIC-Lab

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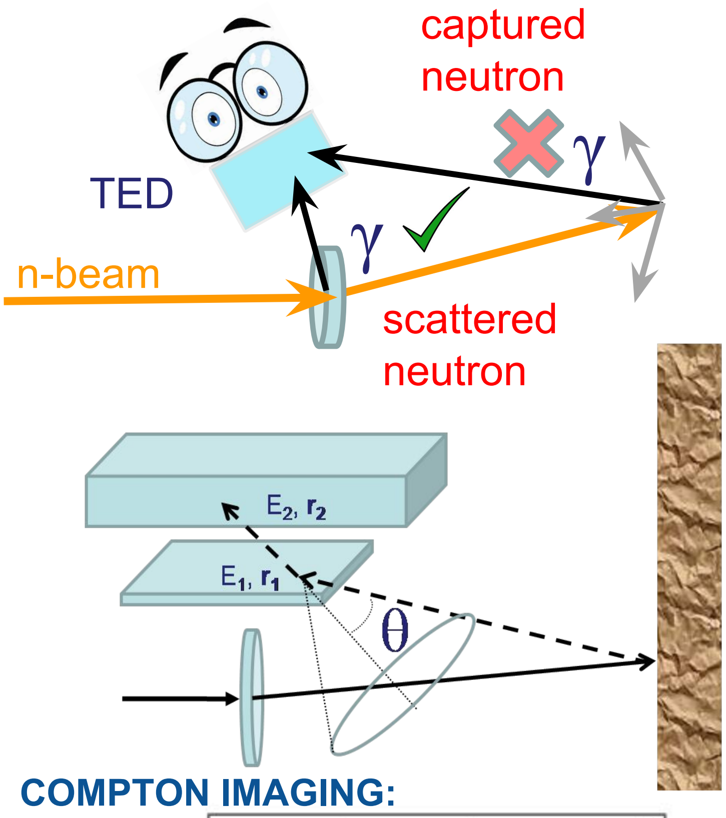

$$\theta = arcos\left(1 - m_e c^2\left(\frac{1}{E_2} - \frac{1}{E_1 + E_2}\right)\right)$$

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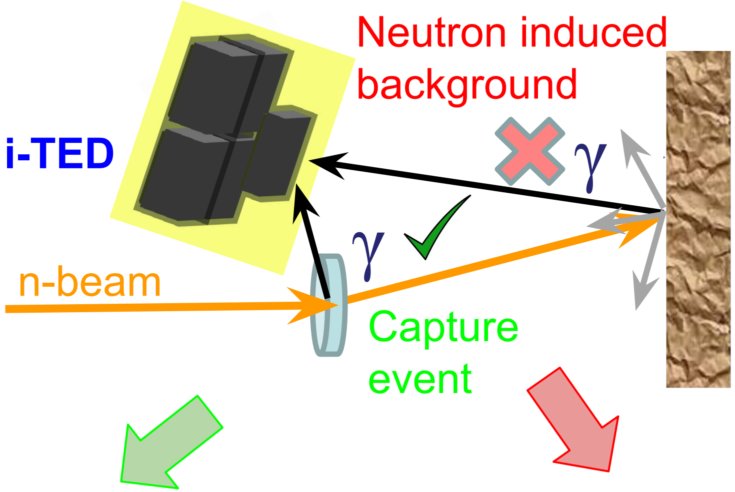
MC simulations of (n,g) and background events

MC Simulation: background rejection

- **MC simulations for capture/background discrimination**



CAPTURE:

CAPTUGEN
Au-197(n,g)

EXTRINSIC BACKGROUND

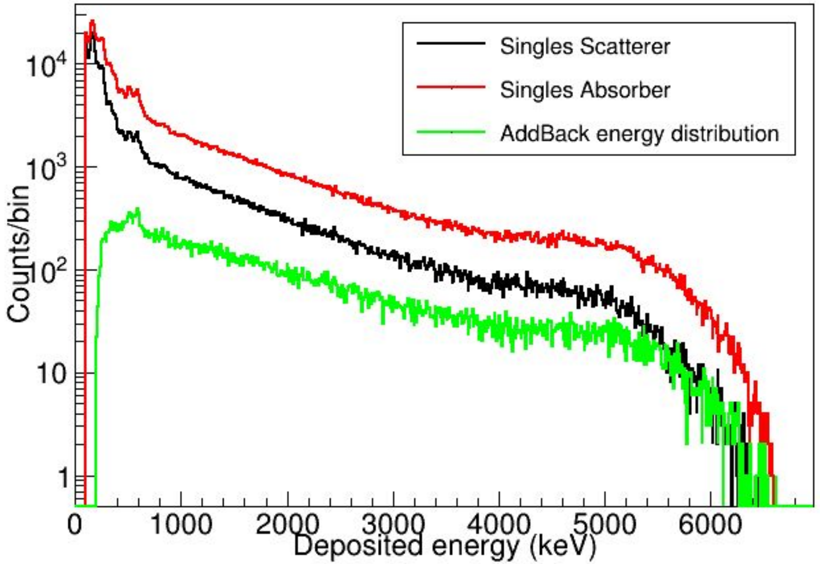
Experimental data
i-TED 5.3
Prototype (2018)

(DETAILS IN BACK-UP)

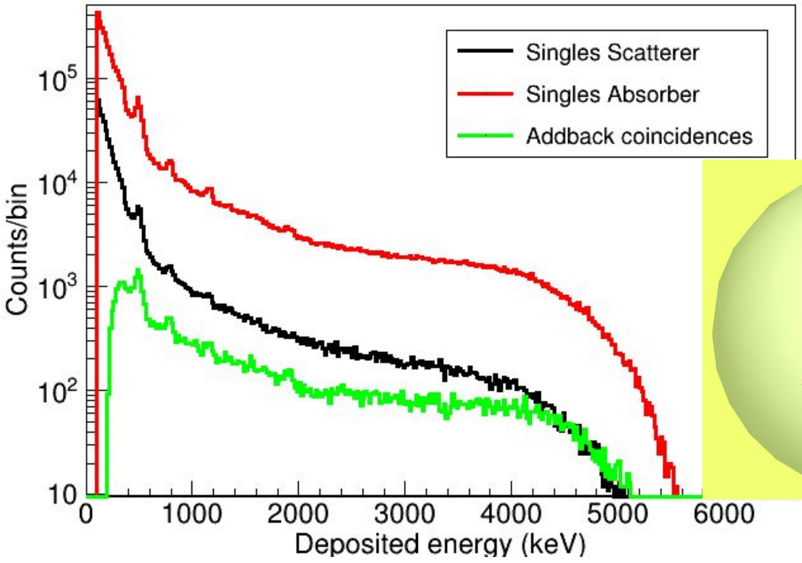
MC i-TED: Response(n,g) & background

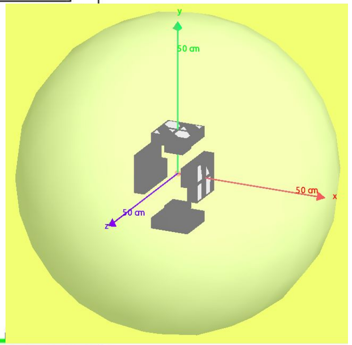
i-TED-5 MC response to (n,g) and background: Singles & coincidences

CAPTURE: Au-197(n,g) (Captugen)



BACKGROUND: Exp. i-TED 5.3 @ EAR1





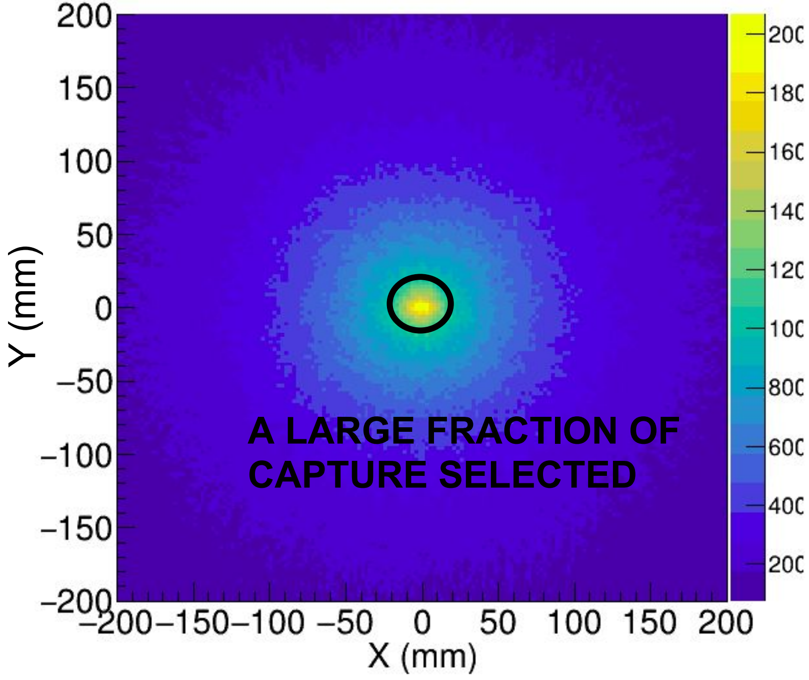
Absorber more affected by extrinsic background from walls + it shields the **scatterer**

Coincidences **(A & S)** reduce more strongly the background →

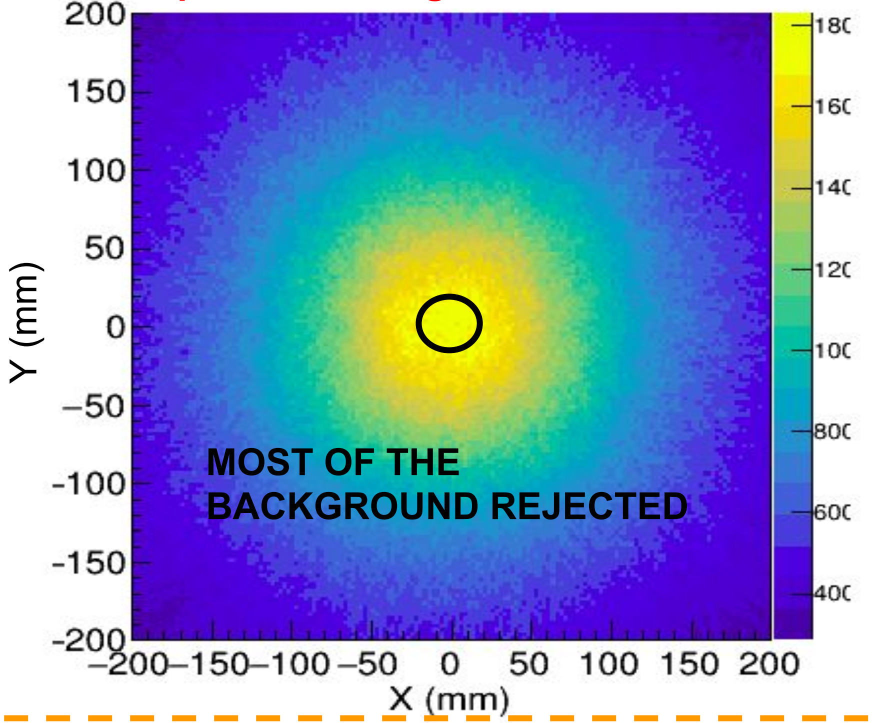
→ **Improved capture/background ratio** before imaging

MC i-TED: imaging (n,g) & background

CAPTURE: Reconstructed emission point for (n,g) events in the sample



BACKGROUND: Reconstructed emission point for background from the walls



i-TED IMAGING OPTIMIZATION : Keep (n,g) efficiency high + Maximum (n,g)/background gain factor

Background rejection based on MC: Imaging and ML algorithms

Imaging cuts using i-TED MC

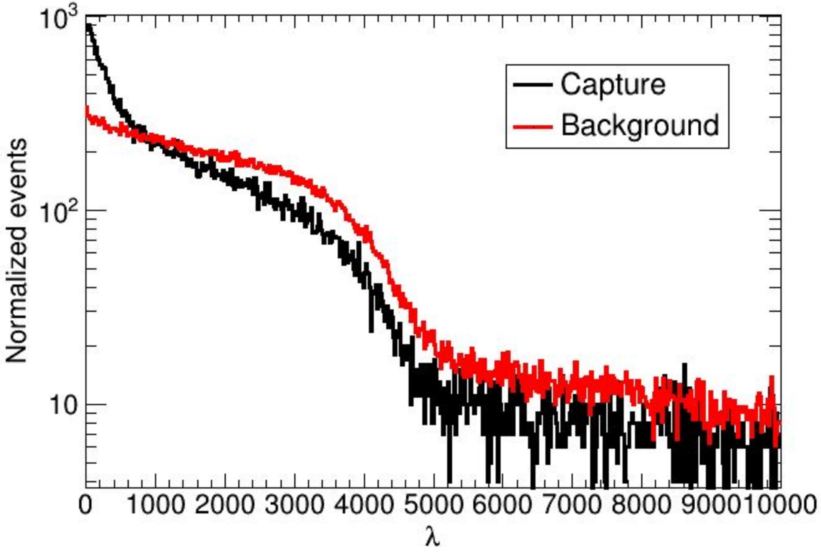
- **Background rejection with imaging cuts: the λ parameter**

Intersection between Compton cone & sample plane

$$\lambda = (n_x a_x + n_y a_y + n_z a_z)^2 - \underbrace{\boxed{(1 + 511/(E_1+E_2) - 511/E_2)^2}}_{\mathrm{Cos}^2(\theta)} (a_x^2 + a_y^2 + a_z^2)$$

Low λ values: γ-rays fulfill the intersection condition between the compton cone and the sample

λ distribution for capture and background (MC)

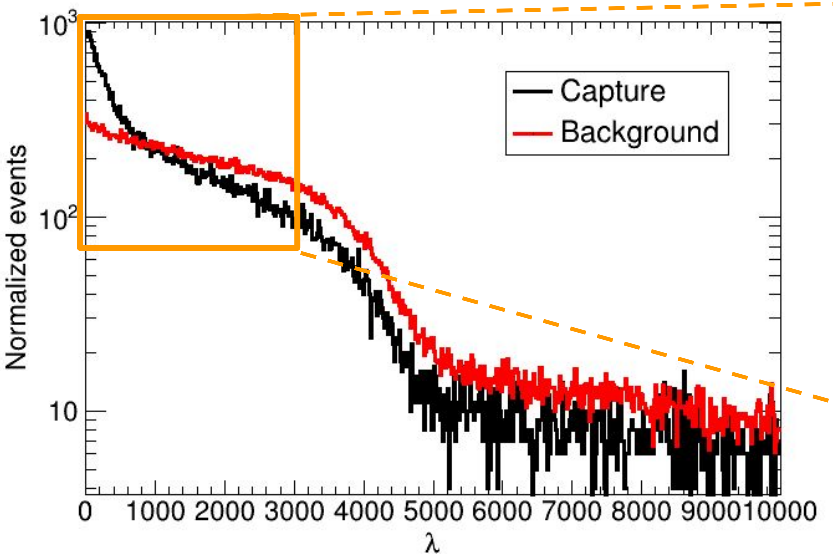


Imaging cuts using i-TED MC

- **Background rejection with imaging cuts: the λ parameter**

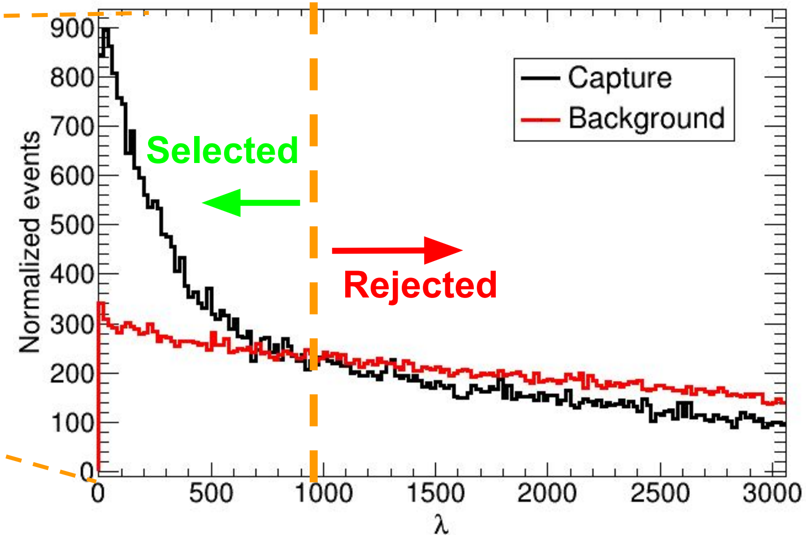
Low λ values: γ-rays fulfill the intersection condition between the compton cone and the sample

λ distribution for capture and background (MC)



Difference between (n,g) and background at Low λ

λ IMAGING CUT



Clear background rejection with λ<500-1000

(n,g)/background: i-TED vs C6D6

MC Results of (n,g)/background: i-TED gain with respect to C6D6

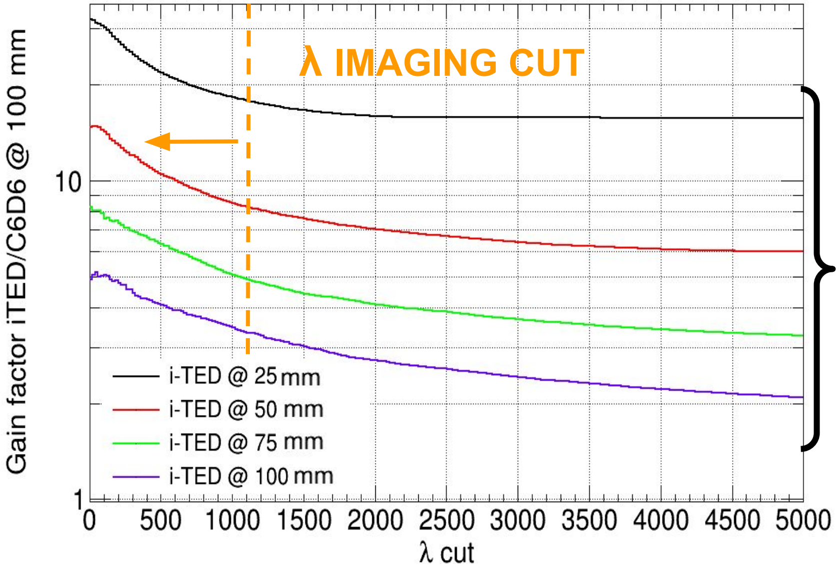
i-TED (n,g)/background gain vs. C6D6:

A) Coincidences crystals: Factor 1.5 – 3 (*)

A) Imaging: Cuts in λ parameter

(*) DETAILS IN BACK-UP

Best gain factors (n, ɣ)/bckg ratio wrt to C6D6



Values with no imaging cut

TOTAL (n,g)/background gain with IMAGING

i-TED gain **factor x 4 - 10**
with respect to a **C6D6 @ 10 cm**
(depending of the sample - i-TED distance)

Cost of THE IMAGING CUTS

(n,g) efficiency reduced to a 20-40%
(for reasonable lambda cuts λ<500-1000)

Background rejection based on MC: ML algorithms vs analytic

ML-based (n,g)/bckg discrimination

- **ML-based capture/background discrimination in a nutshell**

i-TED MC EVENTS:
E1, E2, p1, p2, (t2-t1)

½ CAPTURE

½ BACKGROUND

TRAIN ML-ALGORITHM
XGBoost BINARY CLASSIFIER
(70-80% MC events)

TEST THE ML-ALGORITHM
(Remaining
20-30 % MC events)

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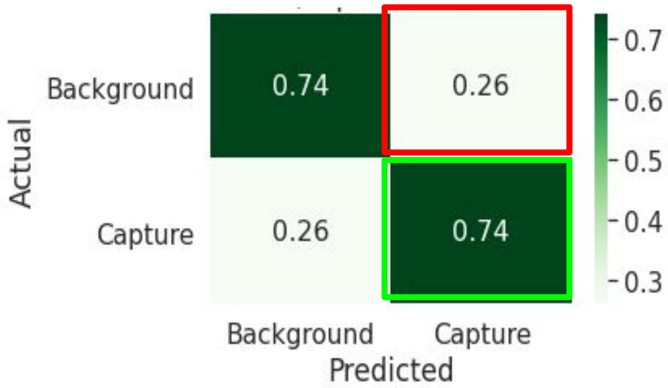
RESULT: CONFUSION MATRIX

FOMs

(n,g) efficiency =
True positive

(n,g)/background
gain factor =
True positive/
False Negative



RESULT WITH IDEAL CRT (MC TIME)

ML-based (n,g)/bckg discrimination

- **ML-based capture/background discrimination in a nutshell**

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½ CAPTURE

½ BACKGROUND

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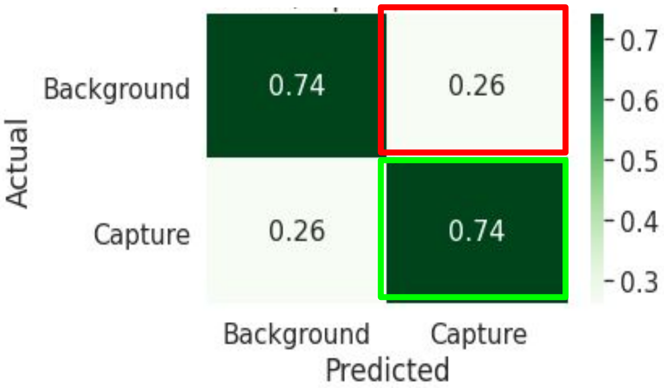


RESULT WITH IDEAL CRT (MC TIME)

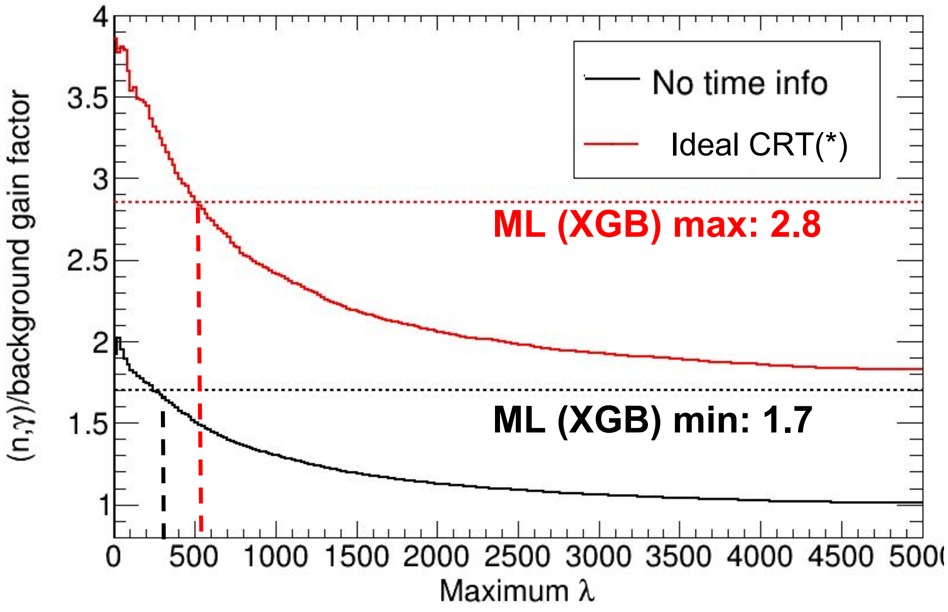
Very promising results

NEXT: compare to imaging cuts

ML-algorithms vs imaging cut (λ)

CAPTURE/BACKGROUND GAIN FACTOR:
ML **(DOTTED)** vs λ Cut **(SOLID)**

(*) Details in the back-up



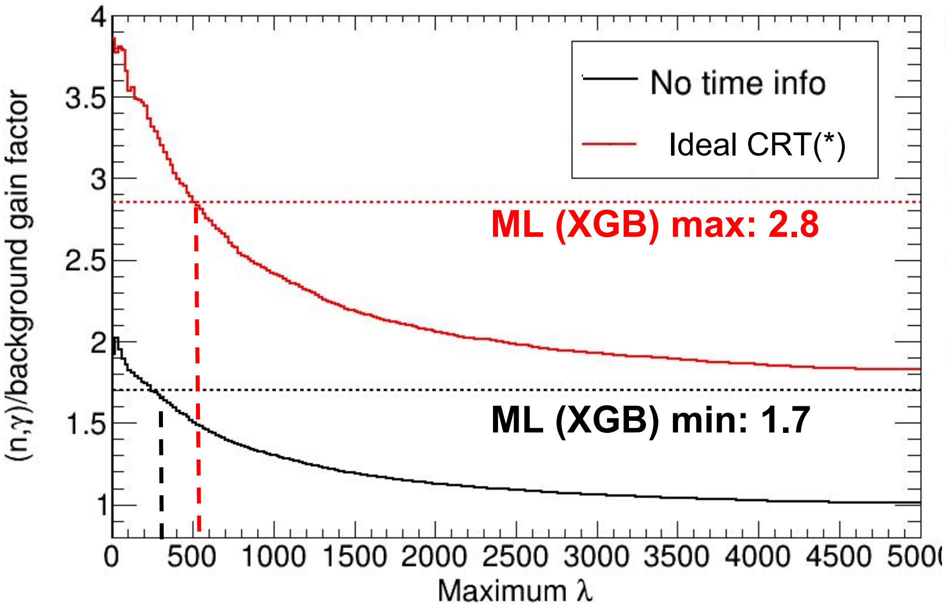
FOM#1:
(n,g)/background gain factor
ML (n,g)/bckg gain factor ~ λ Cut <300-500

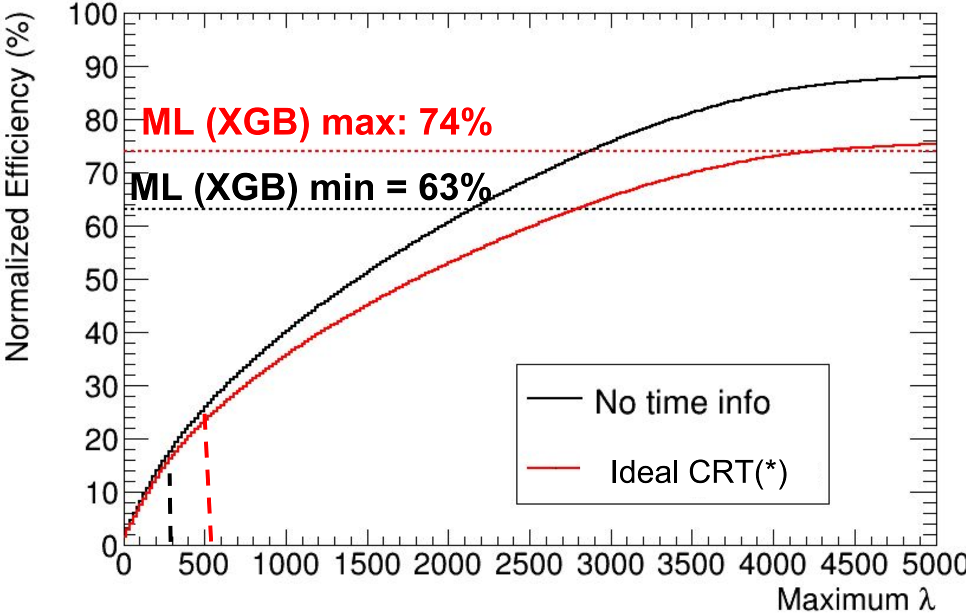
ML-algorithms vs imaging cut (λ)

CAPTURE/BACKGROUND GAIN FACTOR:
ML **(DOTTED)** vs λ Cut **(SOLID)**

(*) Details in the back-up

CAPTURE EFFICIENCY:
ML **(DOTTED)** vs λ Cut **(SOLID)**





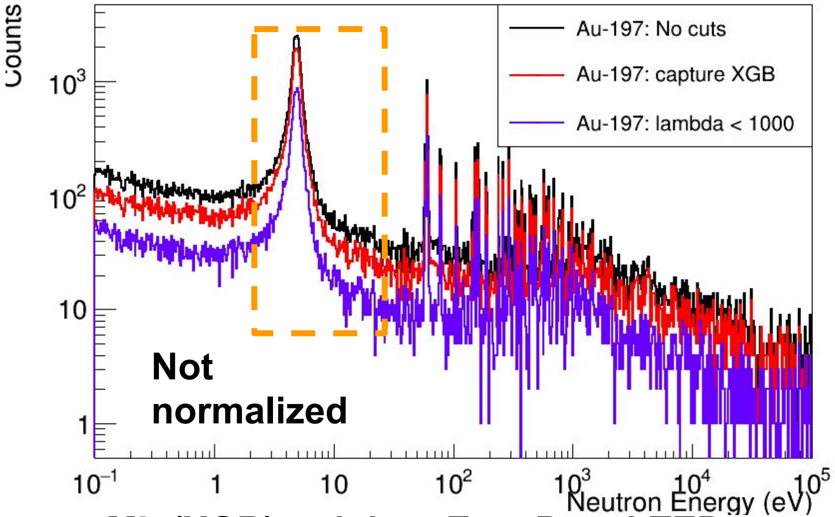
FOM#1:
(n,g)/background gain factor
ML (n,g)/bckg gain factor ~ λ Cut <300-500

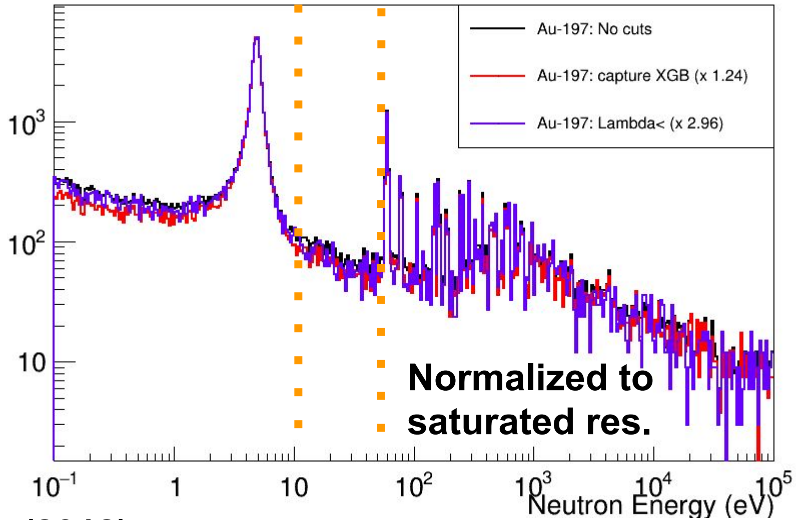
FOM #2: (n,g) efficiency
Same (n,g)/background gain factor
Efficiency ML is x 2-3 LARGER

Background rejection studies based on i-TED 5.3 data

Results ML classifier: Au-197(n,g)

- **ML (n,g)/background (n,g)/bckg classifier: results for Au-197(n,g)**





ML (XGB) training: Exp. Data i-TED prototype (2018)
Au-197 (capture) + Pb (background)

1) **Capture efficiency (4.9 eV res)**

ML (XGB) : 80 %
Analytical λ<1000: 34 %

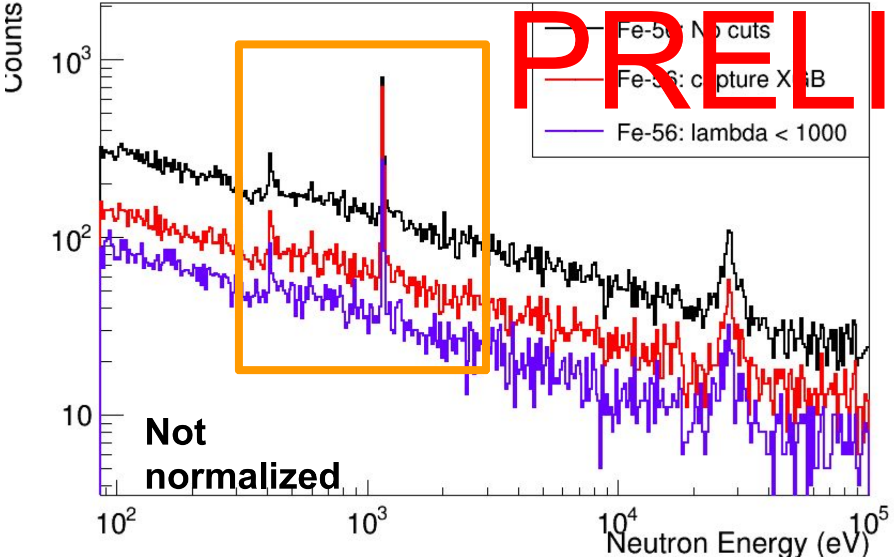
2) **Peak-to-valley gain factor**

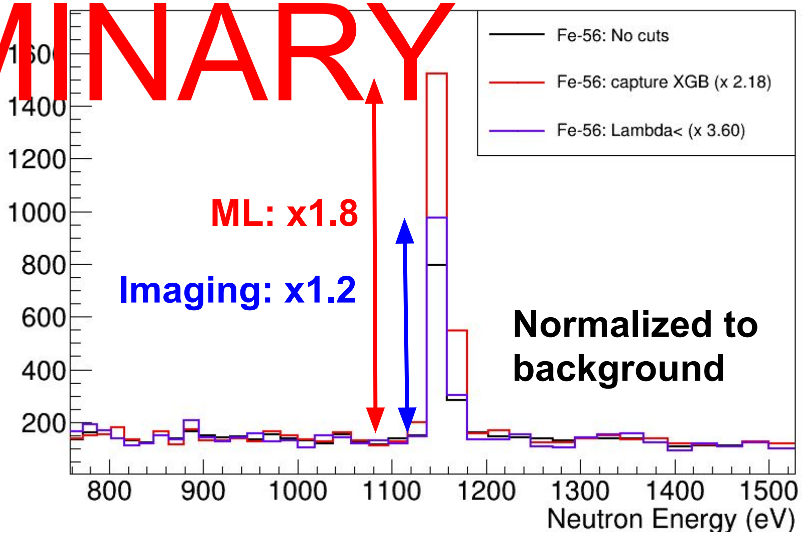
ML (XGB) : 1.24
Imaging λ<1000: 1.14

Au-197: ML provides high (n,g) eff. but background is already low → Fe-56 better to check (n,g)/background gain

Results ML classifier: Fe-56(n,g)

- **ML (n,g)/background (n,g)/bckg classifier: results for Fe-56(n,g)**





ML (XGB) training: Exp. Data i-TED prototype (2018)
Fe-56 (1.15 keV) (capture) + Carbon (background)

1) **Capture efficiency (1.15 keV res)**

ML (XGB) : 80 %
Imaging λ<1000: 32 %

2) **Peak-to-valley gain factor at 1.15 keV**

ML (XGB) : 1.80
Imaging λ<1000: 1.20

Summary

- **i-TED: Imaging techniques to suppress the neutron induced background**

- **Final i-TED 4pi under development and MC simulations are key at this point**
  - Optimization of the (n,g)/background discrimination capabilities
  - Realistic capture and background events

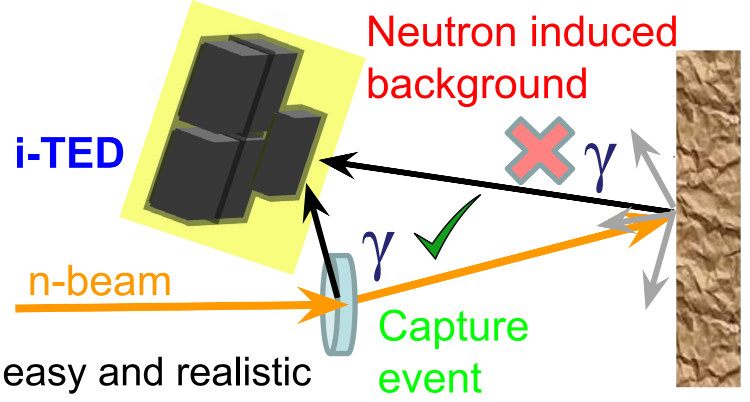
- **Results of (n,g)/background gain factor based on MC**
  - Coincidences + Analytical imaging cuts: i-TED gain factor 4-10 wrt C6D6
  - ML algorithms (XGB) promising: Similar background rejection + x2 (n,g) efficiency

- **ML background rejection with i-TED 5.3 data** (commissioning 2018 EAR1):
  - Training and tested with exp data (Au-197 and Fe-56) → **Preliminary results**
  - Background rejection equal or better than imaging cuts but
  - (n,g) efficiency 2-3 times larger

EXTRA SLIDES
LONG VERSION

MC Simulation: background rejection

- **MC study of capture/background discrimination**
- **Capture events: Au-197(n,g) as a reference**
  - Captugen + Geant4 PrimaryGenerator
- **Neutron induced Background:**
  - Full simulation: Time-cost + (probably) non-realistic
  - Experimental data measured @ EAR1 with i-TED 5.3: easy and realistic



CAPTUGEN Au-197(n,g)

Experimental background i-TED 5.3

(DETAILS IN BACK-UP)

Geant4 Application i-TED 4pi

Output with same structure than exp data

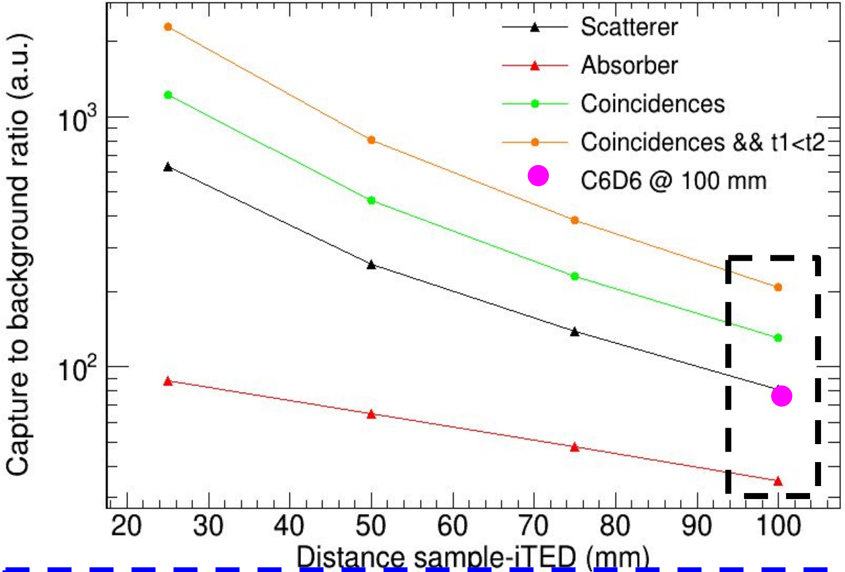
i-TED 5.3 @ EAR1 data

Capture/background discrimination

Analytical Imaging cuts
ML-algorithms

(n,g)/background i-TED vs C6D6

MC Results of (n,g)/background: i-TED gain with respect to C6D6



<u>**(n,g)/background gain BEFORE IMAGING**</u>

Scatterer alone similar to **C6D6**

Gain #1: Coincidences Absorber & Scatter

Gain #2: good CRT & only events with t1<t2

(under study)

Gain (n,g)/background wrt C6D6: x 1.5 - 3

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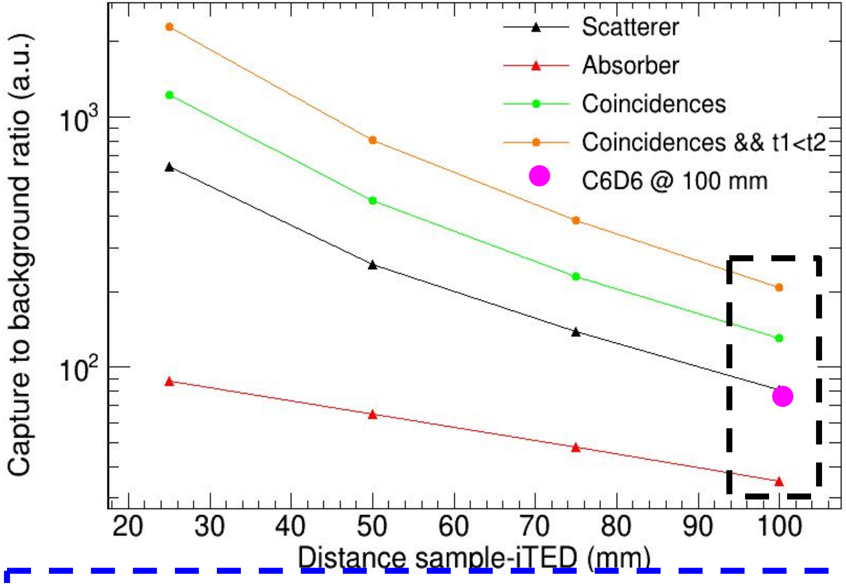

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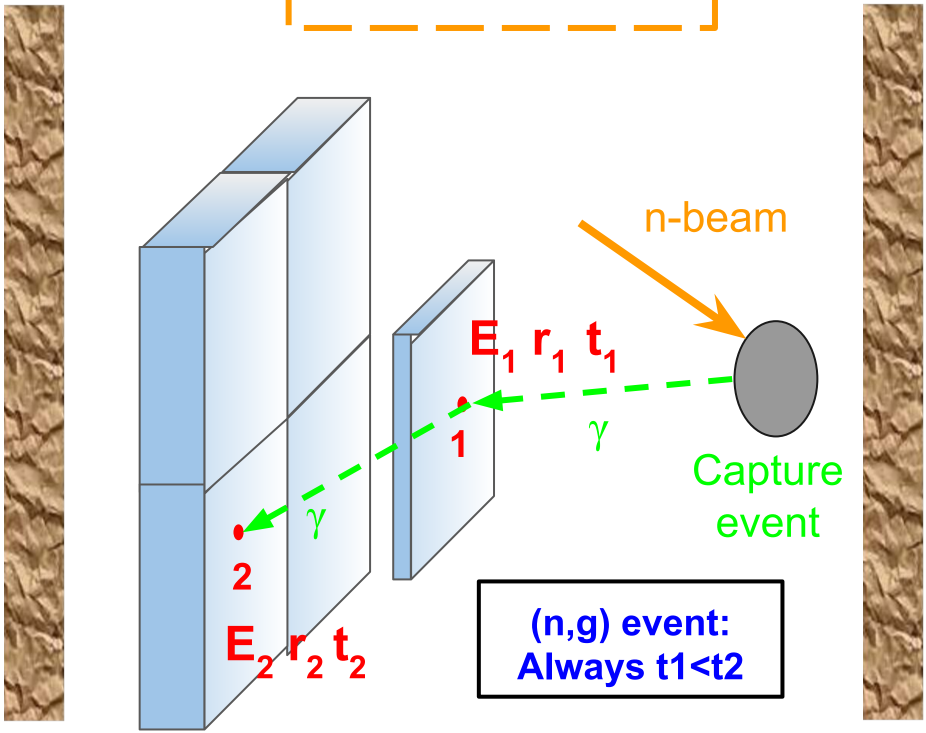
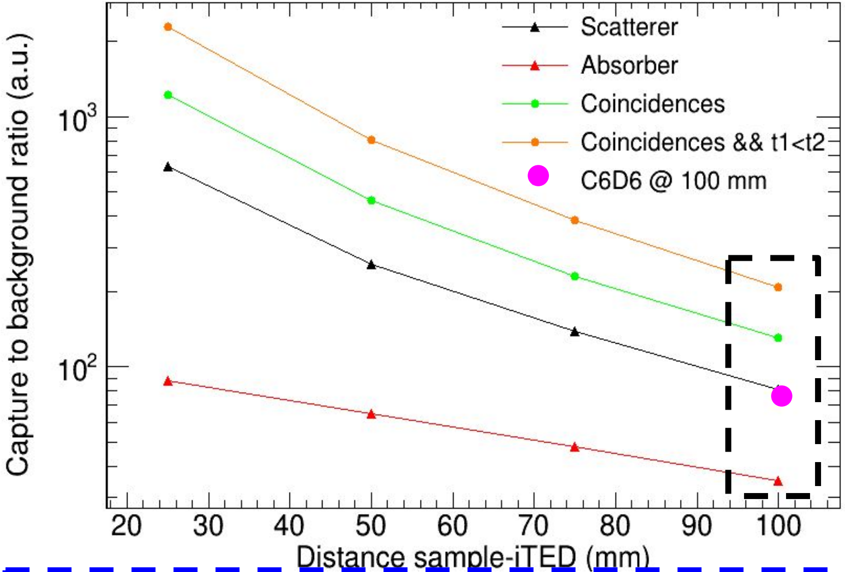


(n,g) event: Always t1<t2

(n,g)/background i-TED vs C6D6

MC Results of (n,g)/background: i-TED gain with respect to C6D6



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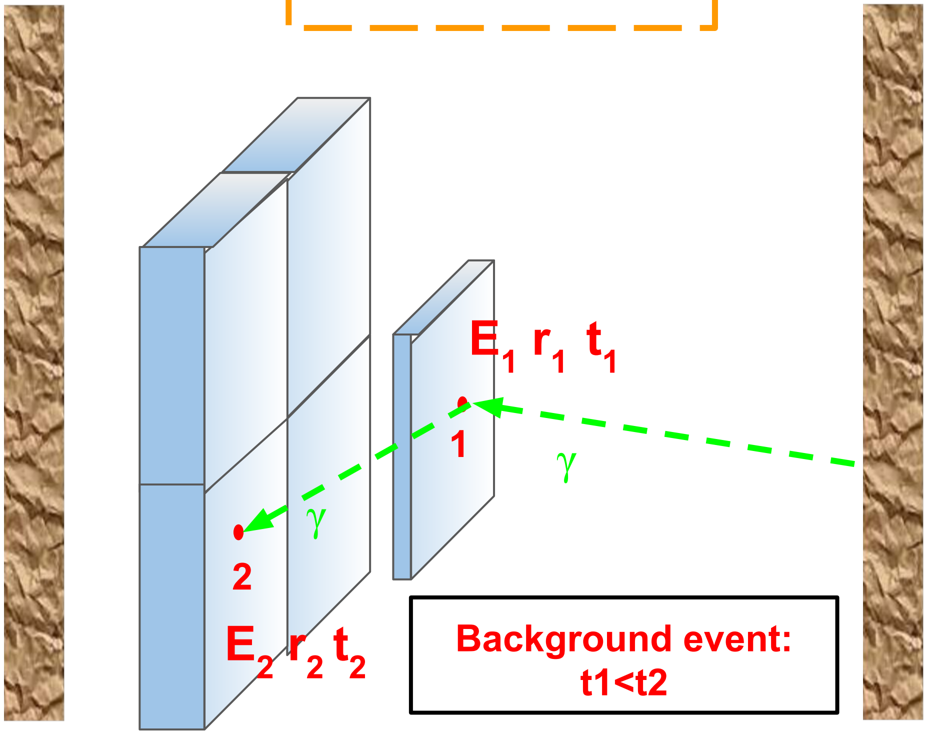

Background event: t1<t2

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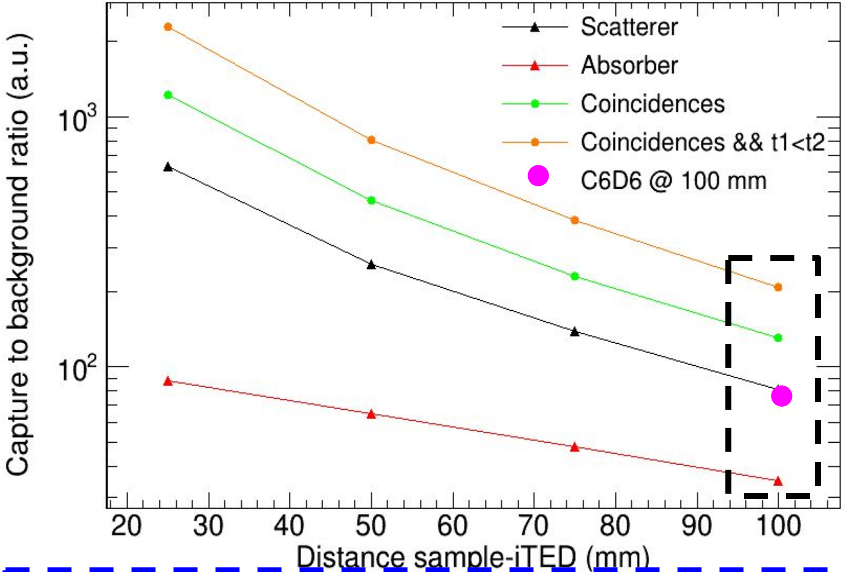

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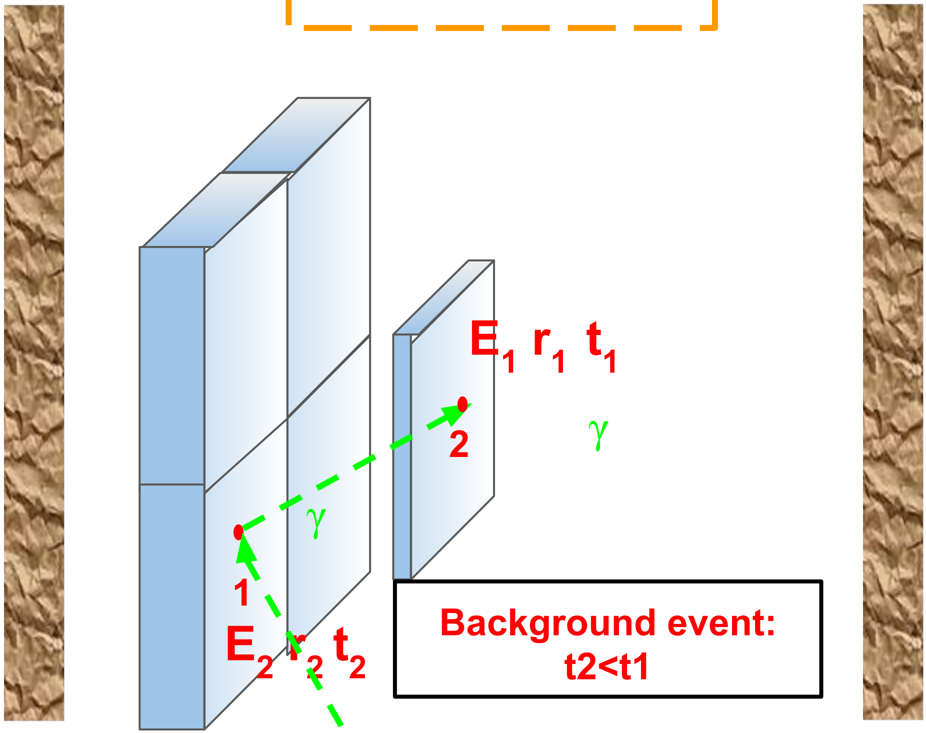

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(n,g)/background i-TED vs C6D6

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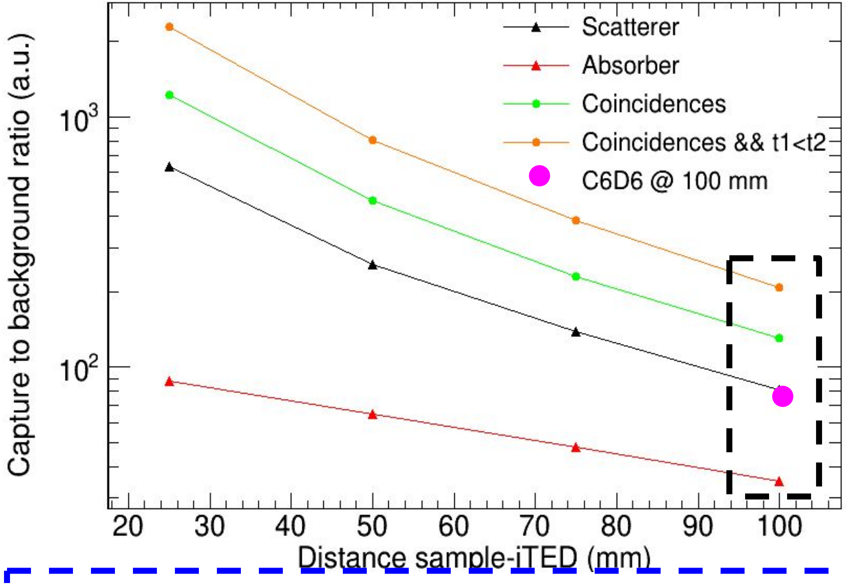

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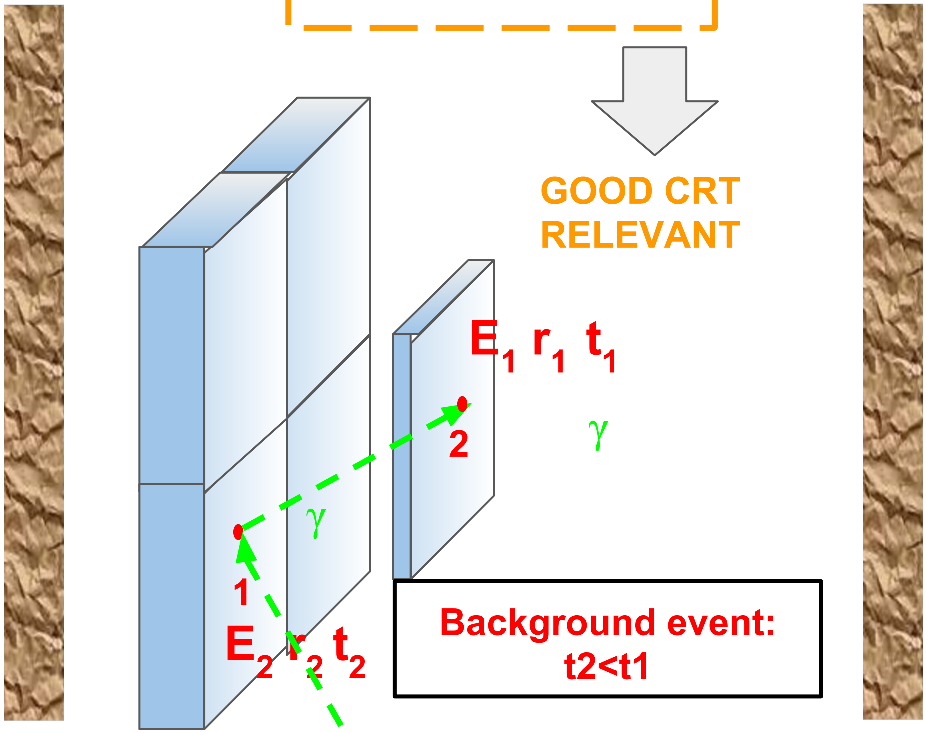
(under study)

Gain (n,g)/background wrt C6D6: x 1.5 - 3

Why Background rejection with t1<t2?

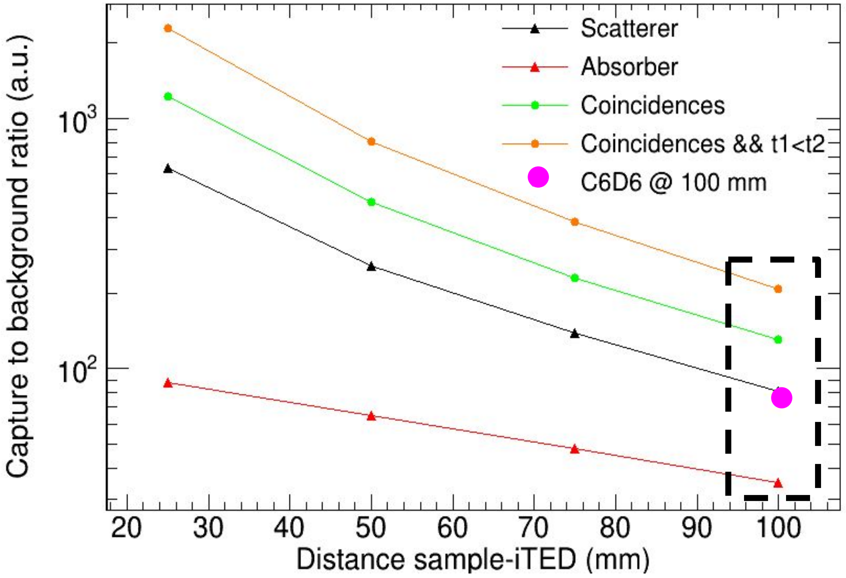
GOOD CRT RELEVANT

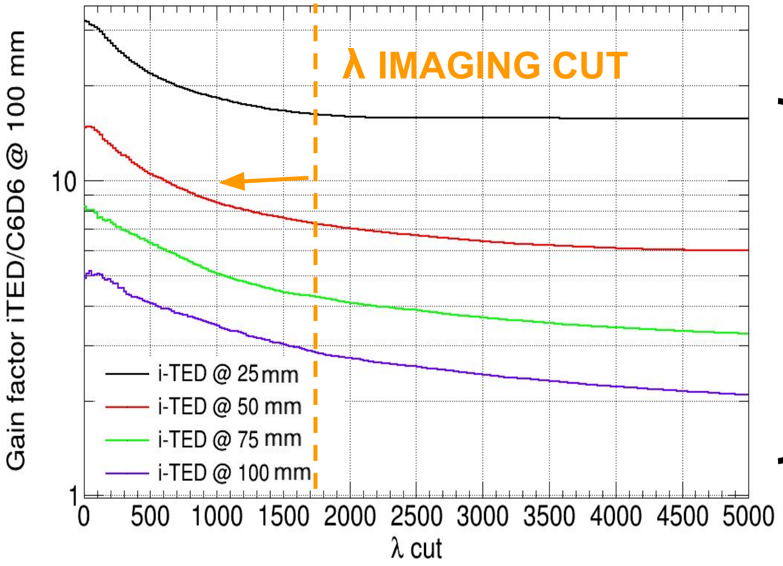


Background event: t2<t1

(n,g)/background i-TED vs C6D6

MC Results of (n,g)/background: i-TED gain with respect to C6D6





Values with no imaging cut

(n,g)/background gain BEFORE IMAGING

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Gain #2: good CRT & only events with t1<t2

(under study)

Gain (n,g)/background wrt C6D6: x 1.5 - 3

TOTAL (n,g)/background gain with IMAGING

i-TED gains a **factor x 4 - 10**

with respect to a **C6D6 @ 10 cm**

depending of the sample - i-TED distance

(Gain related to CRT not included)

ML-based (n,g)/bckg discrimination

- **Binary classifiers: different ML algorithms**
  - **Logistic Regression:** `from sklearn.linear_model import LogisticRegression`
  - **Support Vector Classifier (SVC):** `from sklearn.svm import SVC`
  - **Gaussian Naive Bayes (NB):** `from sklearn.naive_bayes import GaussianNB`
  - **Random Forest:** `from sklearn.ensemble import RandomForestClassifier`
  - **XGBoost Classifier:** `from xgboost import XGBClassifier`
  - **Keras (neural network):** `from tensorflow.keras.models import Sequential`

BEST ACCURACY + SIMPLICITY: XGB

ML-based (n,g)/bckg discrimination

- **ML-based capture/background discrimination in a nutshell**

i-TED MC EVENTS:
9 variables!
Assign a binary flag

1= CAPTURE

0=BACKGROUND

R_E,
R_P,
R_T

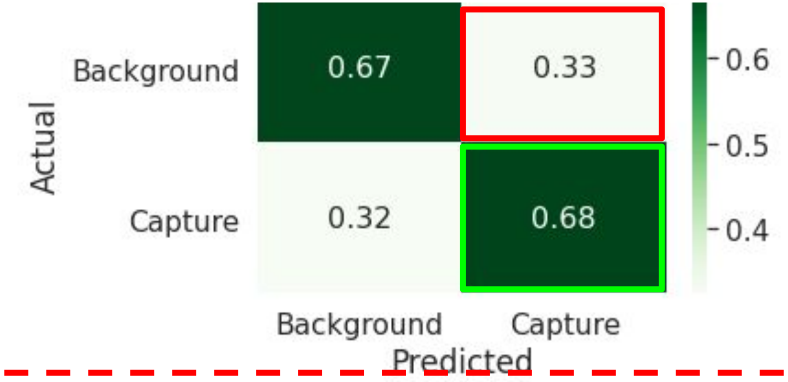
MC + EXP EFFECTS
Energy, Time, Position resolution

BALANCED
N0 EVENTS

TRAIN ML-ALGORITHM BINARY CLASSIFIER (70-80% MC events)

TEST THE ML-ALGORITHM (Remaining 20-30 % MC events)

RESULT: CONFUSION MATRIX



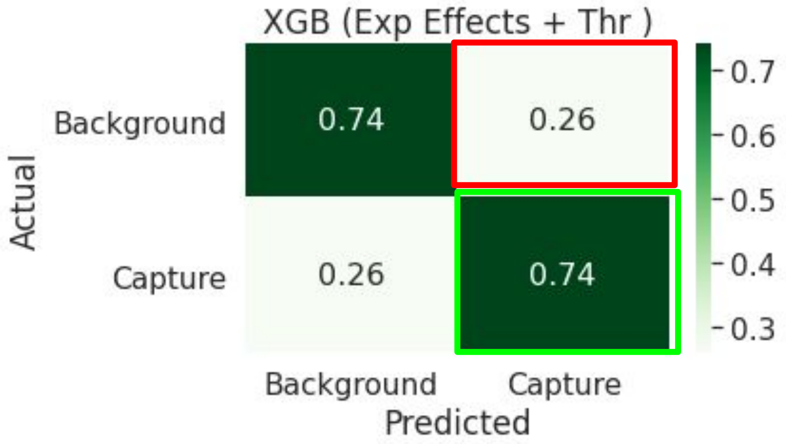
(n,g) efficiency (fraction) =
True positive

(n,g)/background gain factor =
True positive/
False Negative

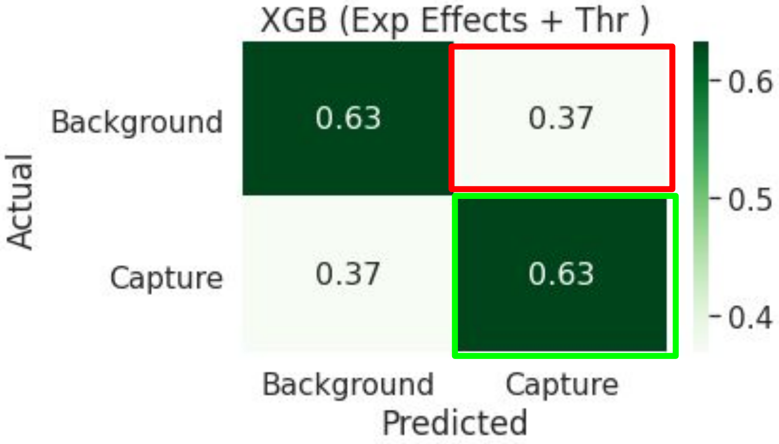
ML-based (n,g)/bckg discrimination

- **ML-based (n,g)/background discrimination: results XGB**

IDEAL CRT (MC TIME):
BEST SCENARIO



DELTA_T NOT INCLUDED:
WORST SCENARIO

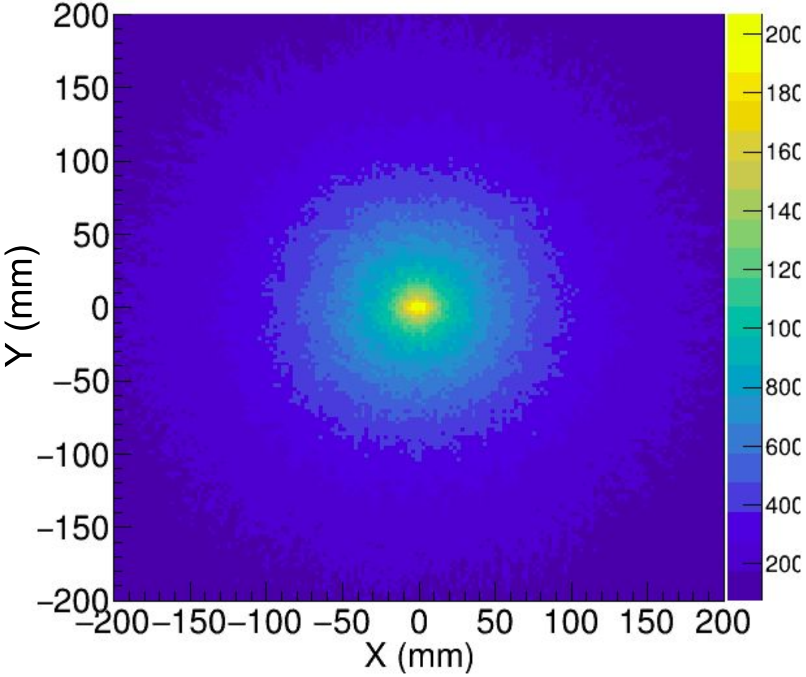


VERY PROMISING RESULTS:

- Background reduced to **26-37%** of the original level
- Capture efficiency kept high: **63-74%** of events
- **Experimental situation** between both results: Depends on CRT but also on the scatter-absorber and detector-sample distance

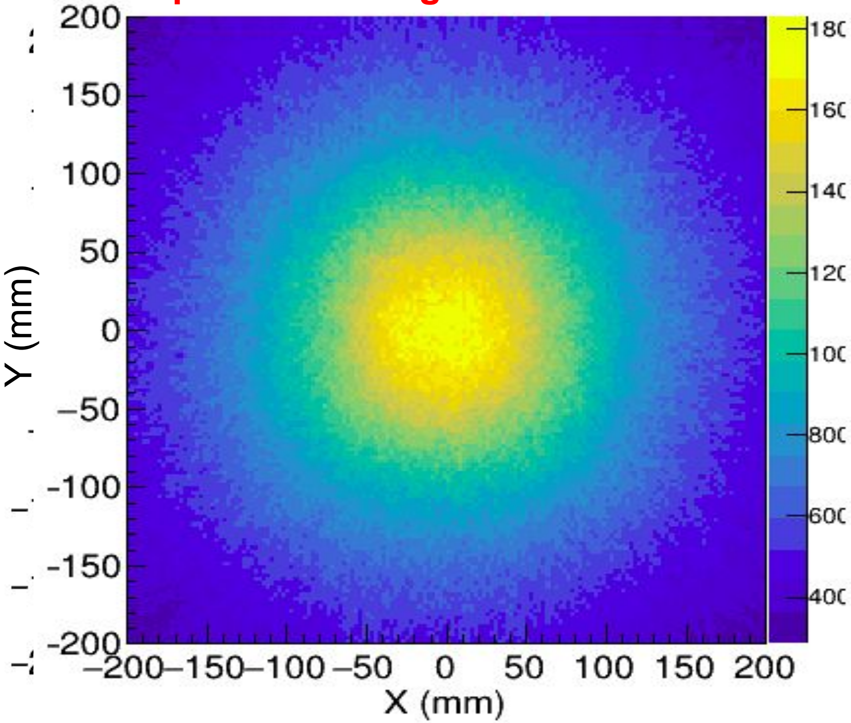
Imaging i-TED: (n,g) & background

CAPTURE: Reconstructed emission point for (n,g) events in the sample



Most of the reconstructed events concentrated around the sample position

BACKGROUND: Reconstructed emission point for background from the walls



The distribution is much flatter with a broader maximum

ML-algorithms vs imaging cut (λ)

TAKE HOME MESSAGE::
Background rejection based in MC events shows very promising results for ML-Algorithms

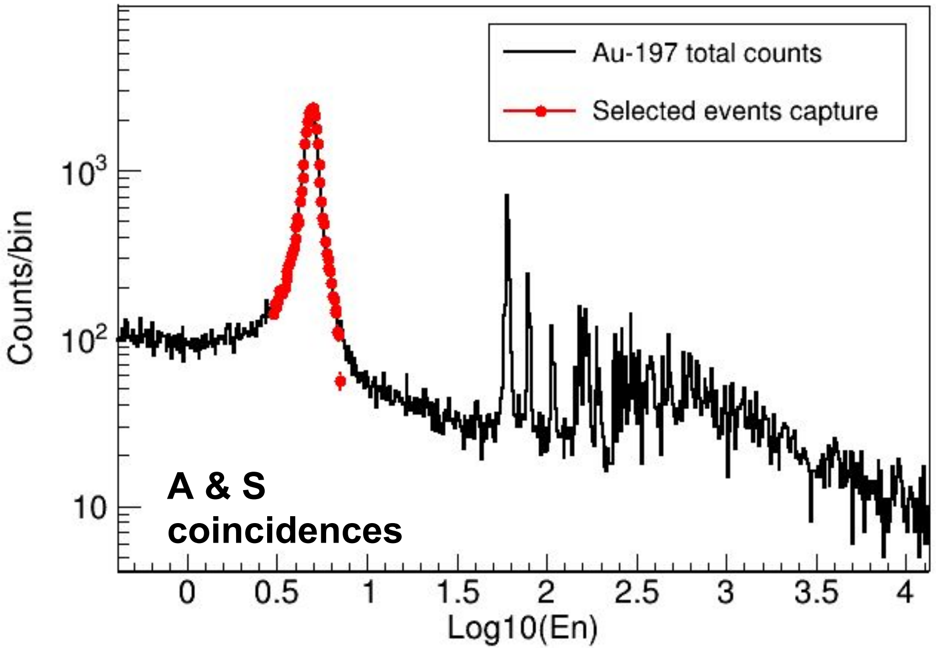
High rejection of background

Larger (n,g) efficiency than imaging cuts

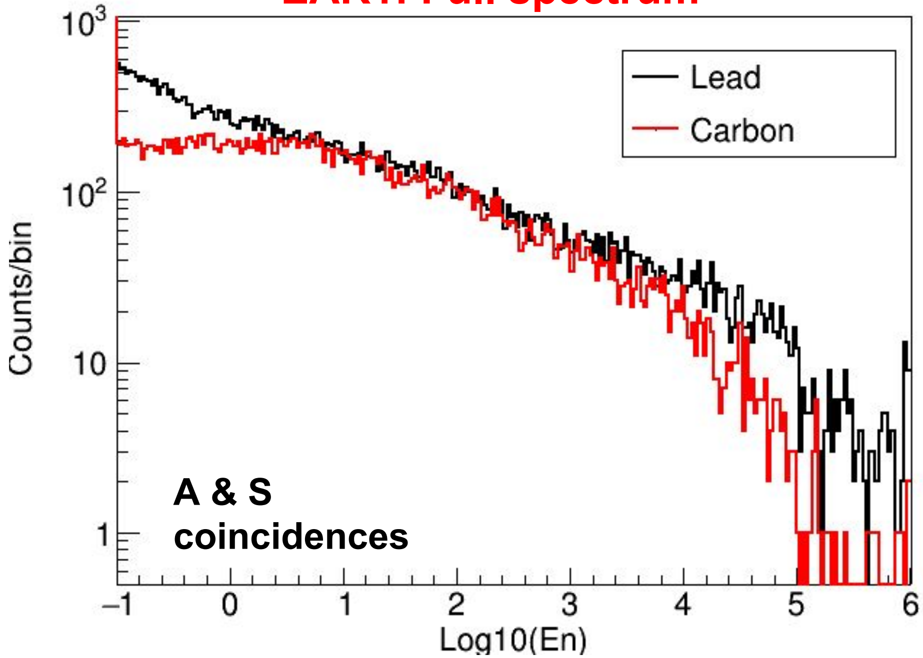
MOTIVATES:
Test ML-algorithms using **exp. Data i-TED 5.3** (prototype commissioning (2018)
(V. Babiano's talk for more details)

ML training: (n,g) and background

CAPTURE: Au-197(n,g)/Fe-56(n,g) i-TED 5.3 @ EAR1



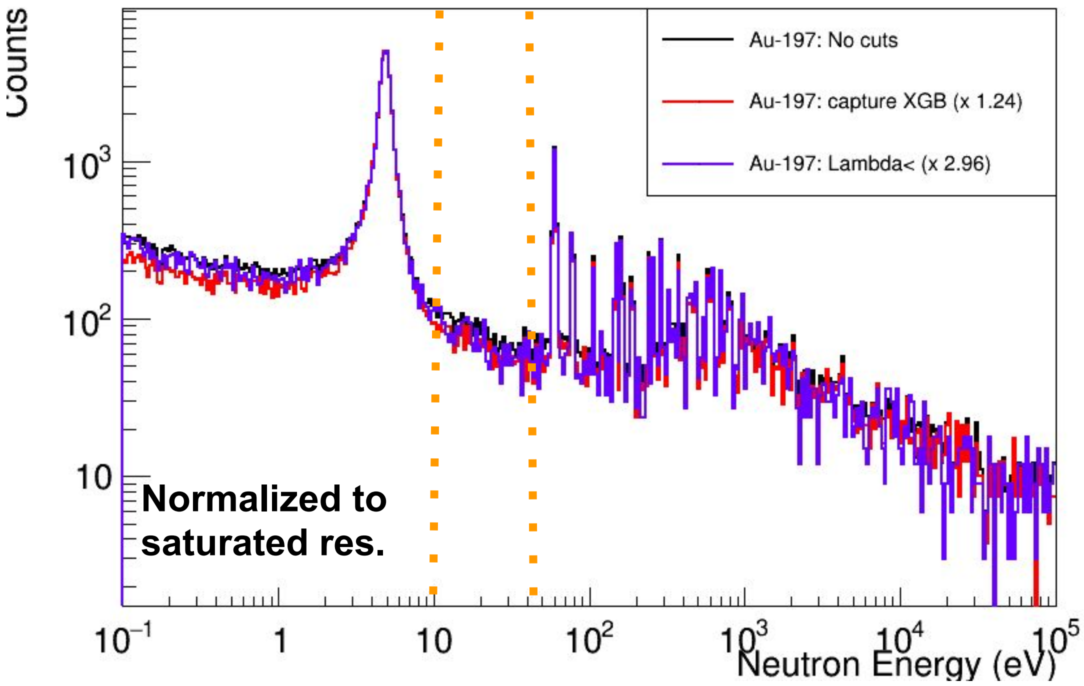
BACKGROUND: Pb/C with i-TED 5.3 @ EAR1: Full spectrum



SAME ML ALGORITHM: **XGBoost** (Best performance in MC-based study)
Same training/testing procedure but replacing the MC input with exp. data

Results ML classifier: Au-197(n,g)

- **ML (n,g)/background (n,g)/bckg discrimination applied to Au-197(n,g)**



ML (XGB) training:
Au-197 (capture) + Pb (background)

Results of the ML-Classifier on Au-197(n,g)

1) **Capture efficiency (4.9 eV res)**

ML (XGB) : 80 %
Imaging λ<1000: 34 %

1) **Peak-to-valley gain factor**

ML (XGB) : 1.24
Imaging λ<1000: 1.14

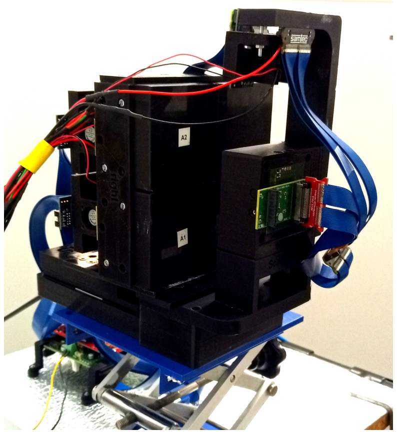
Au-197: ML provides high (n,g) eff. but background is already low → Fe-56 better to check (n,g)/background gain

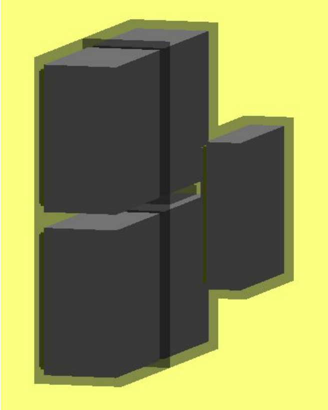
BACK-UP SLIDES

MC simulations i-TED 4π

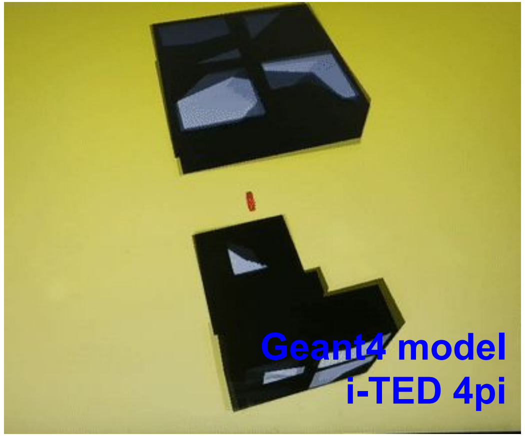
- **Improved existing Geant4 application** for the response of the full i-TED:
  - Detailed geometry of i-TED 5 @ IFIC-lab
  - Simulation Read-out extended to four independent detectors

- **New simulation read-out** to include:
  - Flexible number of i-TED Modules: 1-4
  - Output: root file with same structure than experimental data (Same imaging codes!)
  - For each event: Egamma, E1, E2, r1,r2, t1, t2 , CoincidenceFlag

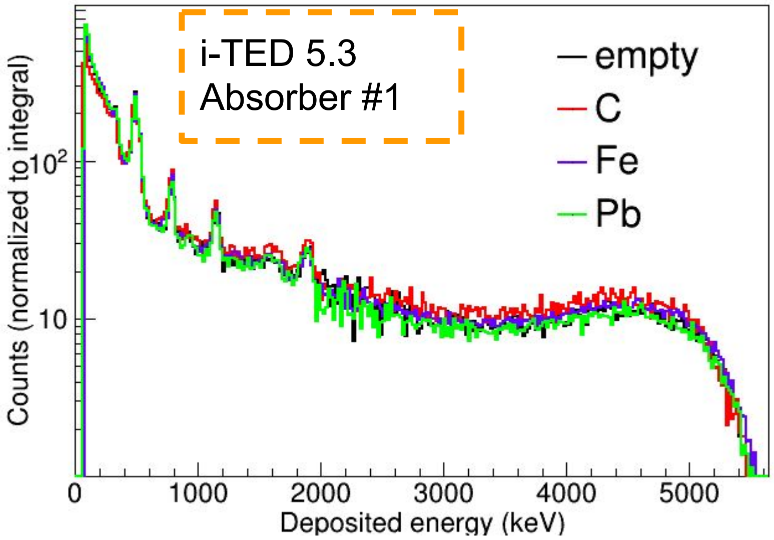


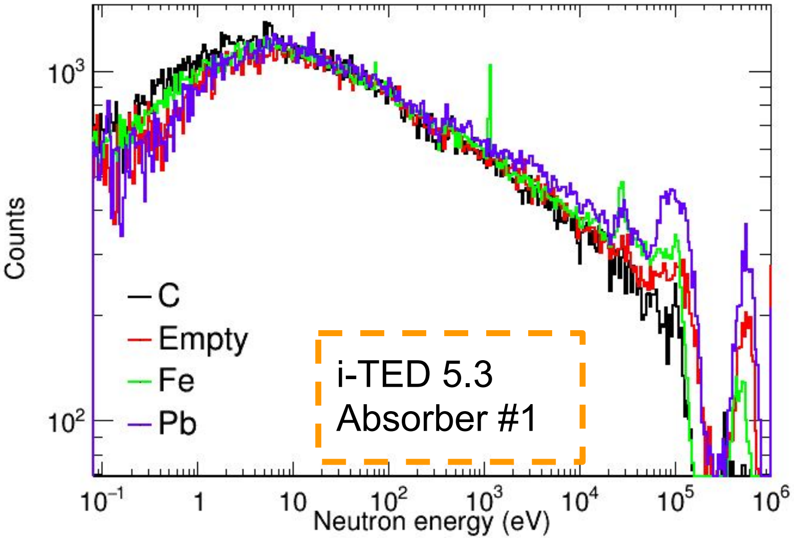


i-TED 5 (each of the modules)



MC Simulation: Background i-TED 5.3

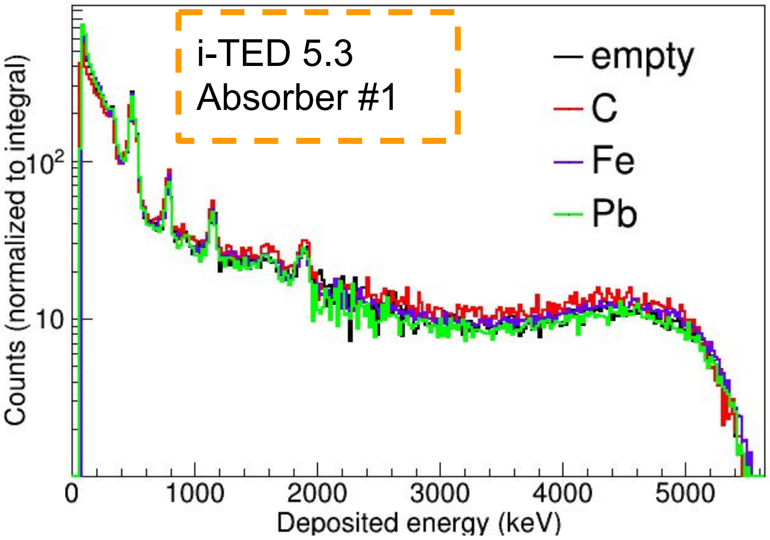


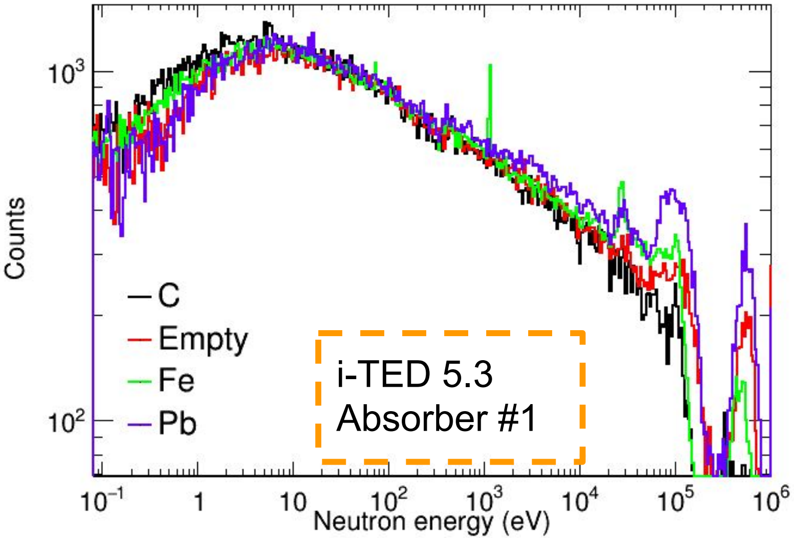


GOAL: Obtain realistic Background due to scattered neutrons

- Background spectra for the MC simulations obtained from **i-TED 5.3 @ EAR1**
- Different samples with large neutron scattering: very similar Edep spectra & TOF spectra → Spectrum **has the same origin for all the samples**
- Studied the impact of i-TED **intrinsic neutron sensitivity** → Negligible!

MC Simulation: Background i-TED 5.3





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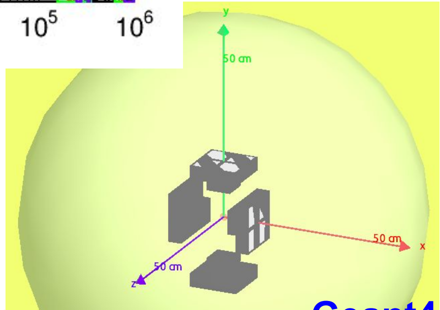
- **Conclusion: Spectra representative of extrinsic background in EAR1**



Geant4 Background sphere R = 0.5 m

i-TED vs C6D6 : (n,g) and activity

C6D6 @ 10 cm vs i-TED: (n,g) Efficiencies

	Eff 1xC6D6 @ 10 cm	
THRESHOLD	Au-197(n,g)	Pu-242(n,g)
100 keV	3.6%	4.5%
150 keV	3.1%	3.6%
250 keV	2.5%	2.7%

Geant4: efficiency 1x Bicron@ 100 mm:

- 3.1 - 3.5 % (thr = 150 keV)
- **2.5 - 2.7% (thr = 250 keV)**

	1 C6D6 @ 100 mm (250 keV Threshold)	1 x I-TED at 100 mm	1x I-TED at 50 mm
Efficiency (n,g)	2.60%	0.20%	0.68%
PbSe activity C. Rate (c/s)	3.04E+04	2.55E+03	8.01E+03
PbSe activity C. Rate with cuts	-	1.50E+03	4.52E+03

Final efficiencies and activity rates for C6D6 and i-TED

	C6D6 @ 100 mm and i-TED @ 100 mm	
C6D6/i-TED (n,g)	C6D6/i-TED activity C Rate	C6D6/i-TED activity w/ cuts
13.0	12.0	20.3
	C6D6 @ 100 mm and i-TED @ 50 mm	
C6D6/i-TED (n,g)	C6D6/i-TED activity C Rate	C6D6/i-TED activity w/ cuts
4	3.8	6.7

Eff ratio C6D6/i-TED:
Scatterer Singles ~ C6D6

Coincidences A & S
x13 if same distance
x4 if i-TED @ 50 mm

Results (n,g)/bckg discrimination ML algorithms

ML-based (n,g)/bckg discrimination

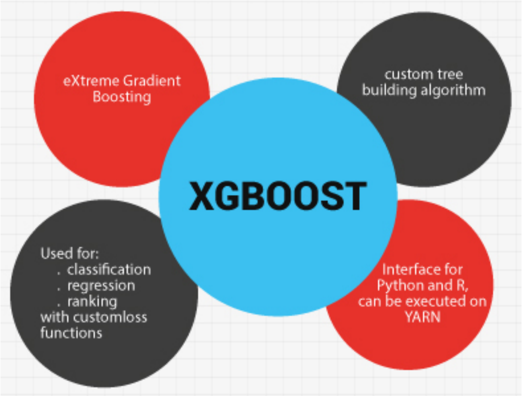
- **Binary classifiers: different ML algorithms**
  - **Logistic Regression:** `from sklearn.linear_model import LogisticRegression`
  - **Support Vector Classifier (SVC):** `from sklearn.svm import SVC`
  - **Gaussian Naive Bayes (NB):** `from sklearn.naive_bayes import GaussianNB`
  - **Random Forest:** `from sklearn.ensemble import RandomForestClassifier`
  - **XGBoost Classifier:** `from xgboost import XGBClassifier`
  - **Keras (neural network):** `from tensorflow.keras.models import Sequential`

BEST ACCURACY + SIMPLICITY: XGB

XGBoost

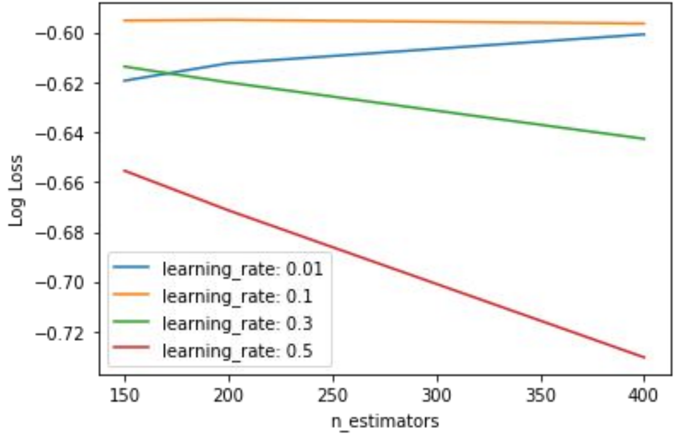
Extreme Gradient Boosting or XGBoost

- Supervised Machine-learning algorithm
- **Goal**: predict a target variable Y given a set of features – Xi.
- **How**: Combines several weak learners into a strong learner to provide a more accurate & generalizable ML model.
- **Multiple applications:** build a regression, binary classification or multi-class classification model.
- **Procedure:** Iterative technique known as boosting that builds a number of decision trees one after the other while focusing on accurately predicting those data points that were not accurately predicted in the previous tree.

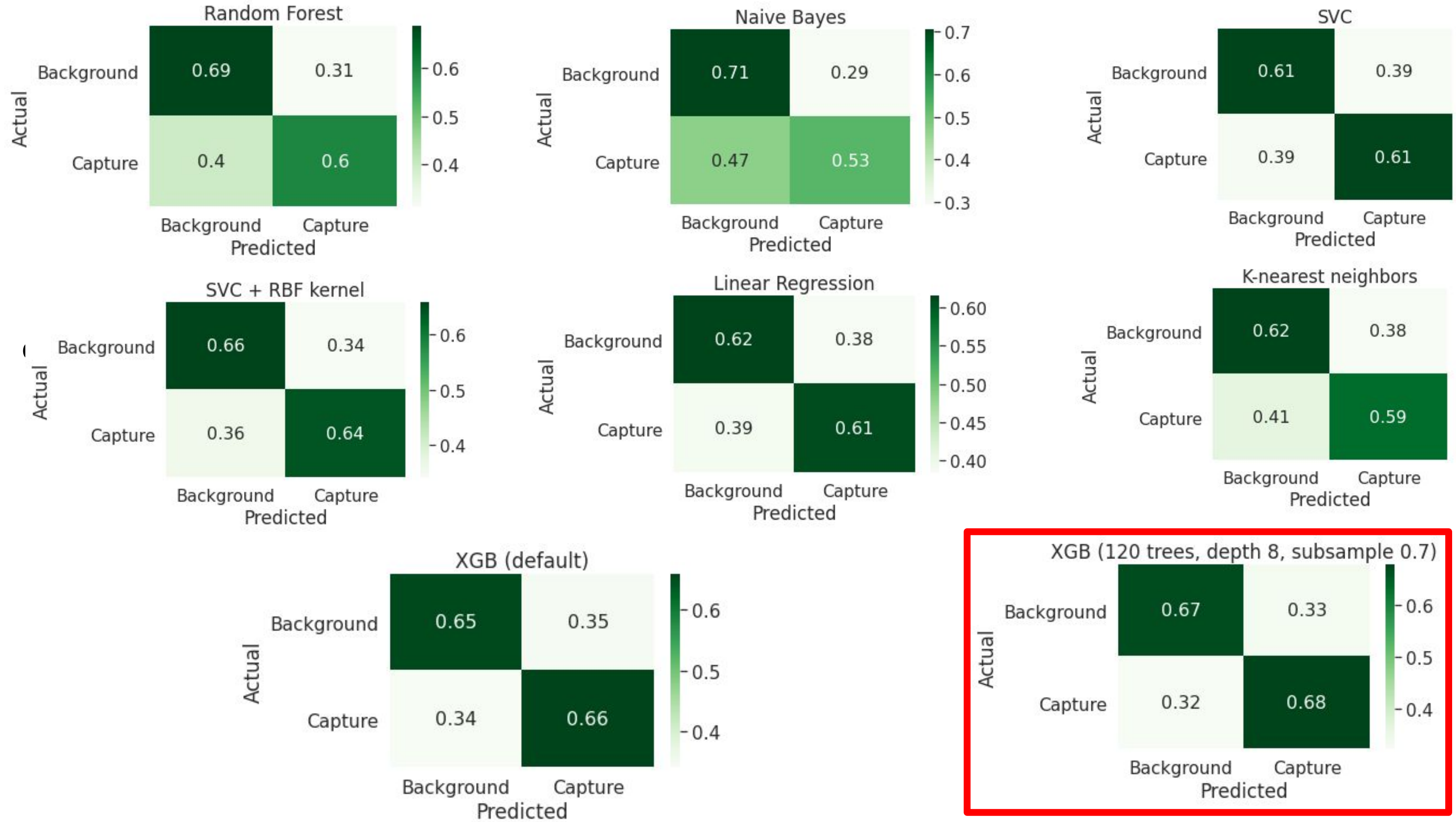


Example of parameter optimization

BEST COMBINATION:
learning_rate= 0.1 &
N_estimators = 150-200



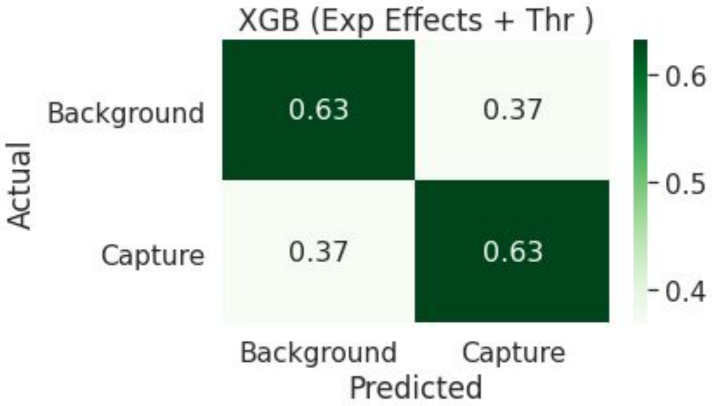
ML bckg rejection

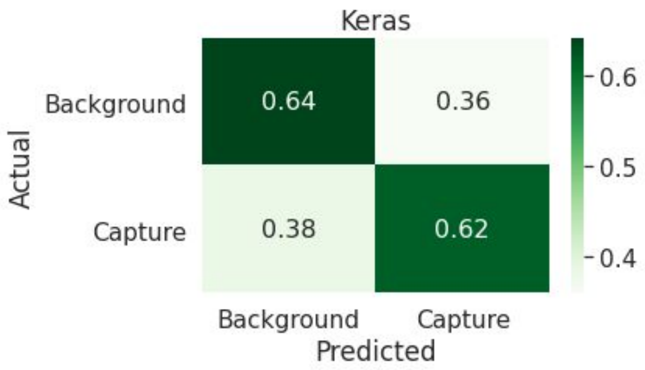


ML background rejection: XGB vs Keras

No delta T
WITH exp. Effects
+ THR

XGB: 63.13%
KERAS: 62.89%



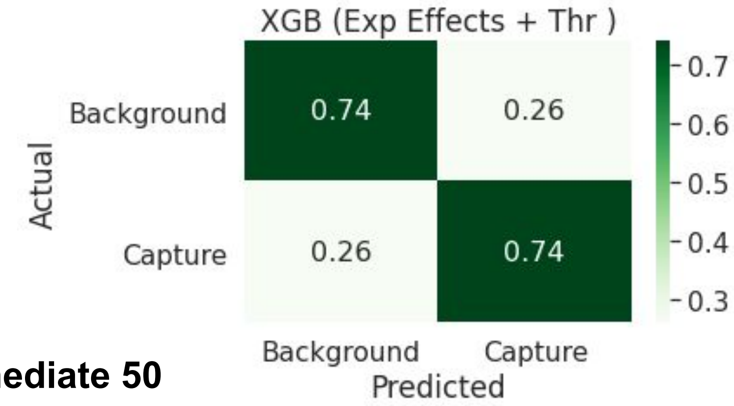


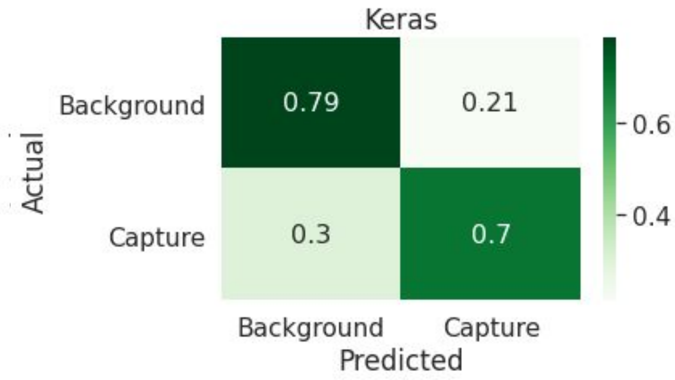
XGB

KERAS (v2)

WITH delta T,
WITH EXP. EFFECTS
+THR

XGB: 73.98%
KERAS: 74.32%



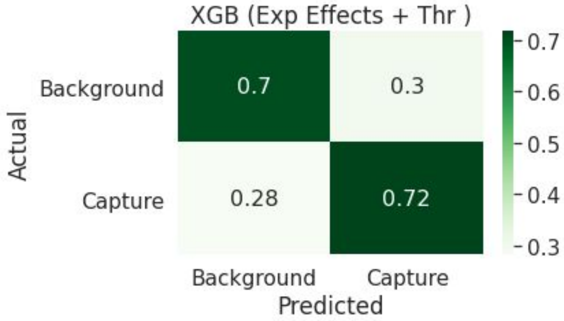


v2) Removed 1 intermediate 50 neurons layer

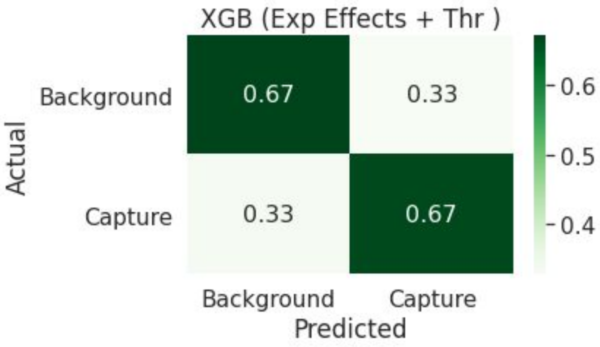
Bckg rejection XGB: impact delta_T

NOW: Realistic resolutions

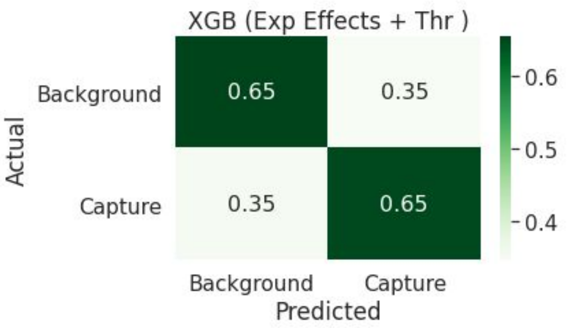
200 ps: 70.98%



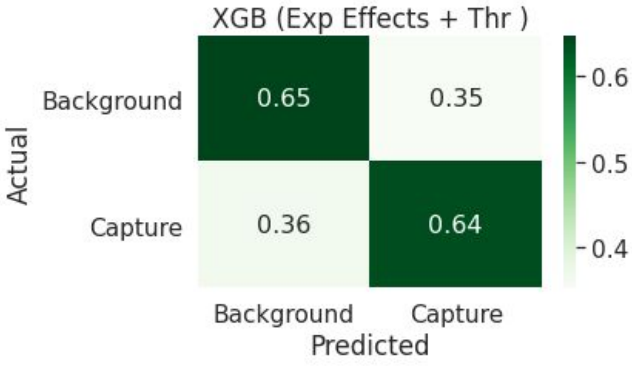
400 ps: 66.94%



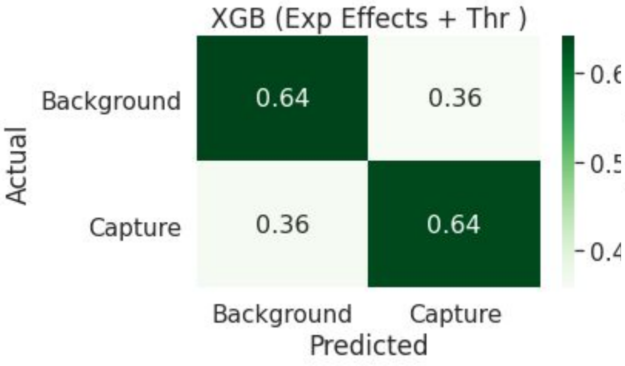
600 ps: 65.10%



800 ps: 64.26%



1000 ps: 63.95%



1200 ps: 63.91%